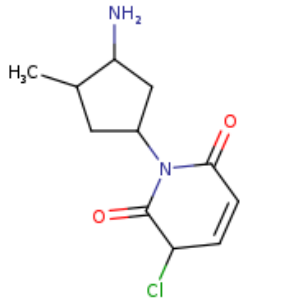
Swiss Institute of Bioinformatics

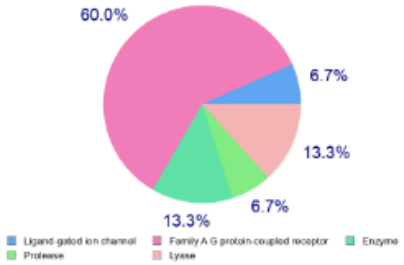
SwissTargetPrediction

Query Molecule



Target Classes

Top 15
Top 25
Top 50
All



Export results:

Show 15 entries

Search:

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Serotonin 3a (5-HT3a) receptor *(by homology)*	HTR3A	P46098	CHEMBL1899	Ligand-gated ion channel		8 / 0
Serotonin 1d (5-HT1d) receptor	HTR1D	P28221	CHEMBL1983	Family A G protein-coupled receptor		3 / 0
Serotonin 1a (5-HT1a) receptor	HTR1A	P08908	CHEMBL214	Family A G protein-coupled receptor		5 / 0
Serotonin 2a (5-HT2a) receptor *(by homology)*	HTR2A	P28223	CHEMBL224	Family A G protein-coupled receptor		30 / 0
Serotonin 2c (5-HT2c) receptor	HTR2C	P28335	CHEMBL225	Family A G protein-coupled receptor		11 / 0
Uridine phosphorylase 1	UPP1	Q16831	CHEMBL4811	Enzyme		4 / 0
Dopamine D2 receptor *(by homology)*	DRD2	P14416	CHEMBL217	Family A G protein-coupled receptor		10 / 0
Aminopeptidase N	ANPEP	P15144	CHEMBL1907	Protease		14 / 0
Beta-1 adrenergic receptor *(by homology)*	ADRB1	P08588	CHEMBL213	Family A G protein-coupled receptor		18 / 0
Beta-glucocerebrosidase	GBA	P04062	CHEMBL2179	Enzyme		14 / 0
Carbonic anhydrase II	CA2	P00918	CHEMBL205	Lyase		8 / 0
Carbonic anhydrase I	CA1	P00915	CHEMBL261	Lyase		2 / 0
Alpha-2a adrenergic receptor	ADRA2A	P08913	CHEMBL1867	Family A G protein-coupled receptor		4 / 0
Alpha-2b adrenergic receptor *(by homology)*	ADRA2B	P18089	CHEMBL1942	Family A G protein-coupled receptor		3 / 0
Alpha-1a adrenergic receptor	ADRA1A	P35348	CHEMBL229	Family A G protein-coupled receptor		7 / 0

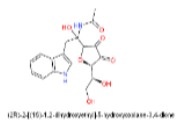
Showing 1 to 15 of 100 entries

6:38

Draw

Local | Cloud

Tags | Filter



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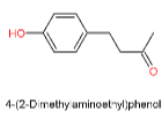

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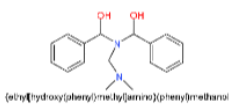

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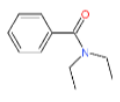

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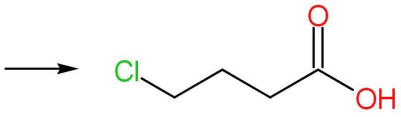
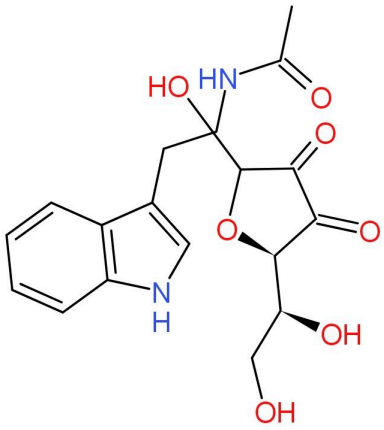
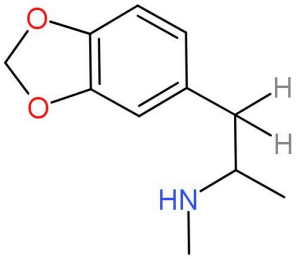
Draw | Work | Msg | Me



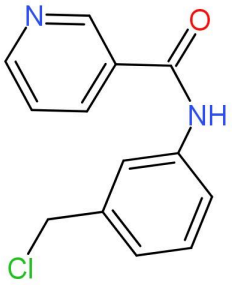
4-aminobutanoicacid chloride



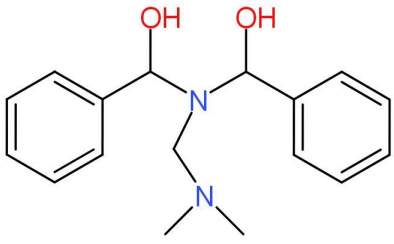
(2R)-2-[(1S)-1,2-dihydroxyethyl]-5-hydroxyoxolane-3,4-dione



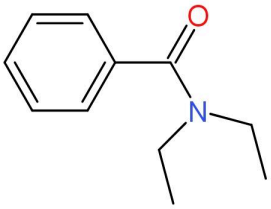
[1-(2H-1,3-benzodioxol-5-yl)propan-2-yl](methyl)amine



N-[3-(chloromethyl)phenyl]pyridine-3-carboxamide



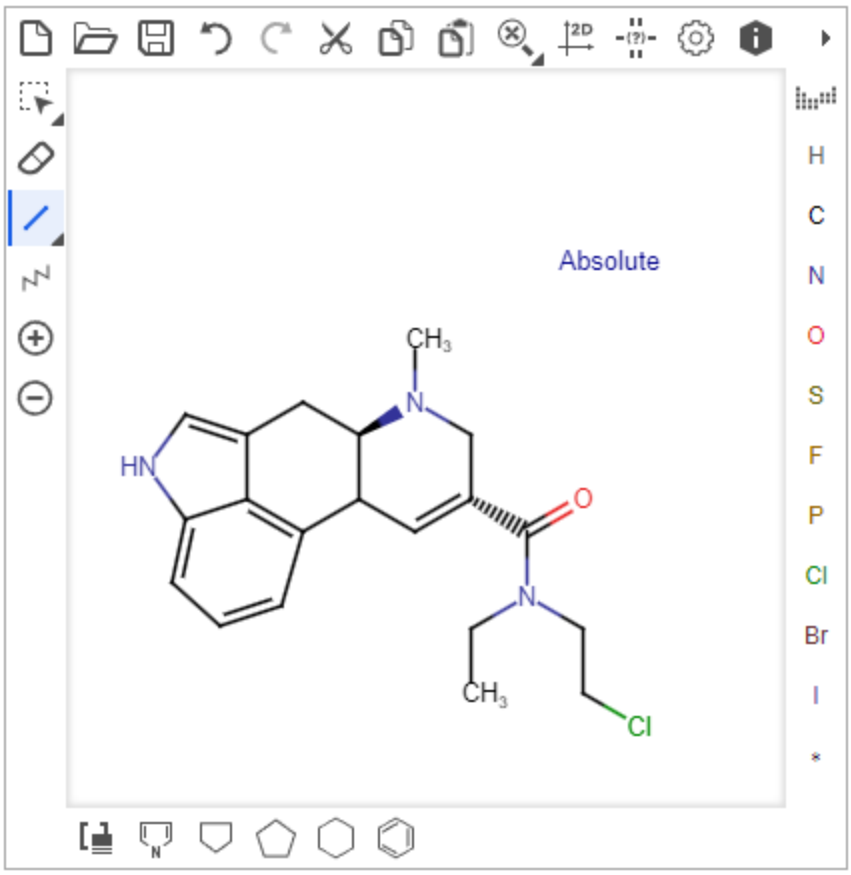
{ethyl[hydroxy(phenyl)methyl]amino}(phenyl)methanol



N,N-diethylbenzamide

Zoete, V., Daina, A., Bovigny, C., & Michielin, O. SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening., *J. Chem. Inf. Model.*, **2016**, *56(8)*, 1399-1404

CCN(CCCl)C(=O)C1=CC2[C@@H](CC3=CNC4=CC=CC2=C34)N(C)C1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CH3
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CH3
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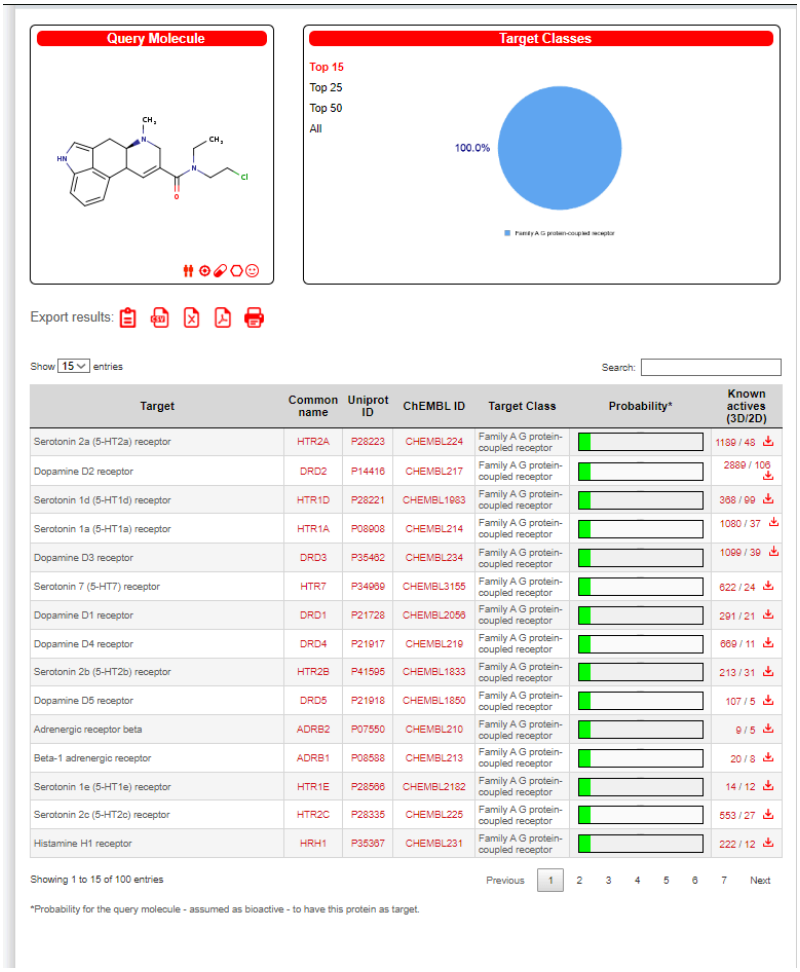
Query Molecule
Target Classes
Top 15
Top 25
Top 50
All
100.0%
Export results:
Show 15 entries
Search:
Target | Common name | Uniprot ID | ChEMBL ID | Target Class | Probability* | Known actives (3D/2D)
Serotonin 2a (5-HT2a) receptor | HTR2A | P28223 | CHEMBL224 | Family A G protein-coupled receptor | 1189 / 48
Dopamine D2 receptor | DRD2 | P14416 | CHEMBL217 | Family A G protein-coupled receptor | 2889 / 106
Serotonin 1d (5-HT1d) receptor | HTR1D | P28221 | CHEMBL1983 | Family A G protein-coupled receptor | 368 / 99
Serotonin 1a (5-HT1a) receptor | HTR1A | P08908 | CHEMBL214 | Family A G protein-coupled receptor | 1080 / 37
Dopamine D3 receptor | DRD3 | P35462 | CHEMBL234 | Family A G protein-coupled receptor | 1099 / 39
Serotonin 7 (5-HT7) receptor | HTR7 | P34969 | CHEMBL3155 | Family A G protein-coupled receptor | 622 / 24
Dopamine D1 receptor | DRD1 | P21728 | CHEMBL2056 | Family A G protein-coupled receptor | 291 / 21
Dopamine D4 receptor | DRD4 | P21917 | CHEMBL219 | Family A G protein-coupled receptor | 669 / 11
Serotonin 2b (5-HT2b) receptor | HTR2B | P41595 | CHEMBL1833 | Family A G protein-coupled receptor | 213 / 31
Dopamine D5 receptor | DRD5 | P21918 | CHEMBL1850 | Family A G protein-coupled receptor | 107 / 5
Adrenergic receptor beta | ADRB2 | P07550 | CHEMBL210 | Family A G protein-coupled receptor | 9 / 5
Beta-1 adrenergic receptor | ADRB1 | P08588 | CHEMBL213 | Family A G protein-coupled receptor | 20 / 8
Serotonin 1e (5-HT1e) receptor | HTR1E | P28566 | CHEMBL2182 | Family A G protein-coupled receptor | 14 / 12
Serotonin 2c (5-HT2c) receptor | HTR2C | P28335 | CHEMBL225 | Family A G protein-coupled receptor | 553 / 27
Histamine H1 receptor | HRH1 | P35367 | CHEMBL231 | Family A G protein-coupled receptor | 222 / 12
Showing 1 to 15 of 100 entries
Previous 1 2 3 4 5 6 7 Next
*Probability for the query molecule - assumed as bioactive - to have this protein as target.

OC1CCC(C1)N1CCC2=CC=CC(=C2)C1=O

Vitolidine